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Teller's Contributions to Atomic and Molecular Physics

January 15, 2008, marks the 100th anniversary of Edward Teller's birth. This highlight is the seventh in a series of 10 honoring his life and contributions to science.

EDWARD Teller kept a small statue in his Livermore office of the Greek philosopher Democritos. Born about 460 B.C., Democritos advanced an early concept of atomic theory when, at one of Plato's seminars, he proposed that the universe was composed of two indivisible elements: the atom and the void.

At the dawn of the 20th century, scientists continued to question the existence of atoms. Atomic theory worked well in chemistry, but it conflicted with the well-established classical laws of physics. The birth of quantum mechanics in the 1920s provided the theoretical framework needed to study atomistic behavior. The powerful physical picture and mathematical tools of quantum mechanics allowed physicists, including Teller, to describe the behavior of atoms and molecules and explain, often for the first time, phenomena that previously puzzled them.

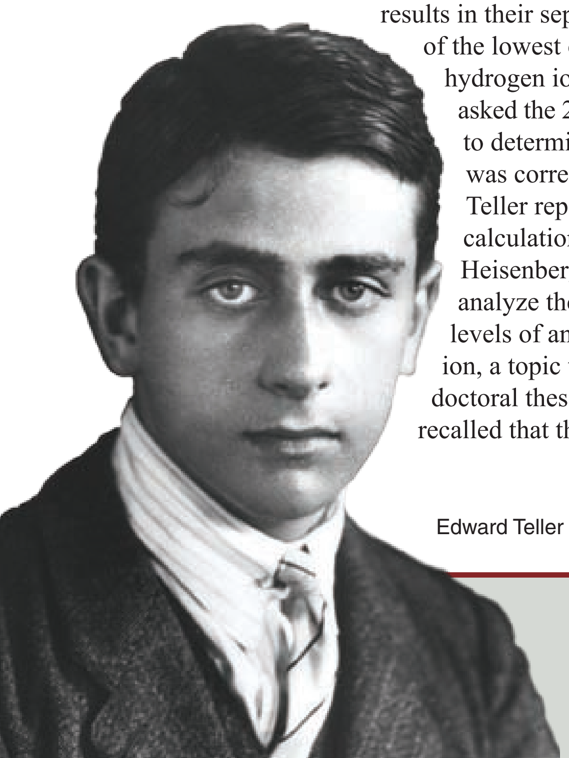
Teller studied quantum mechanics at the University of Leipzig under Werner Heisenberg, a major contributor to the theory. At this time, scientists did not completely understand even the simplest molecule—the hydrogen ion, which has two protons and one electron in a bound state. The theories being proposed to explain the molecule's behavior often contradicted each other.

For example, two physicists, Carl Jensen Burrau of Denmark and A. H. Wilson from the U.S., derived different results in their separate calculations of the lowest energy state for the hydrogen ion. In 1929, Heisenberg asked the 20-year-old Teller to determine which result was correct. A few days later, Teller reported that Burrau's calculation was accurate. Heisenberg then had Teller analyze the higher energy levels of an excited hydrogen ion, a topic that became Teller's doctoral thesis. In *Memoirs*, Teller recalled that the project involved "lots of busy work, a little diligence, and no originality." It also required him to use a noisy calculating machine in a room below Heisenberg's living quarters. According to Teller, Heisenberg declared the thesis work completed when he tired of the machine's racket. The resulting paper, "Hydrogen Molecular Ion," appeared in 1930 in *Zeitschrift für Physik.* It was the first of many in which Teller applied quantum mechanics to molecular physics.

Teller worked with László Tisza, a friend from Hungary, on another molecular physics problem. In this project, the two physicists examined the spectral consequences of coupling the nuclear vibration and molecular rotation of a methyl halide molecule. Methyl halide has one carbon atom, three hydrogen atoms, and one atom of a halogen, either iodine, bromine, chlorine, or fluorine. Teller and Tisza extended the Franck–Condon principle, which explains the electronic transitions occurring in a polyatomic molecule as it vibrates and rotates. Their 1932 paper, also published in *Zeitschrift für Physik*, was the first of a series examining how polyatomic molecules behave when, under varying circumstances, the electronic levels cross.

Teller's work on molecular physics culminated in a collaboration with Hermann Jahn. Their 1937 paper, "Stability

The Teller family enjoyed playing chess: (from left) Teller's son, Paul; wife, Mici; daughter, Wendy; and Teller.



Edward Teller graduated from the Minta Model School in Budapest, Hungary, in 1925.

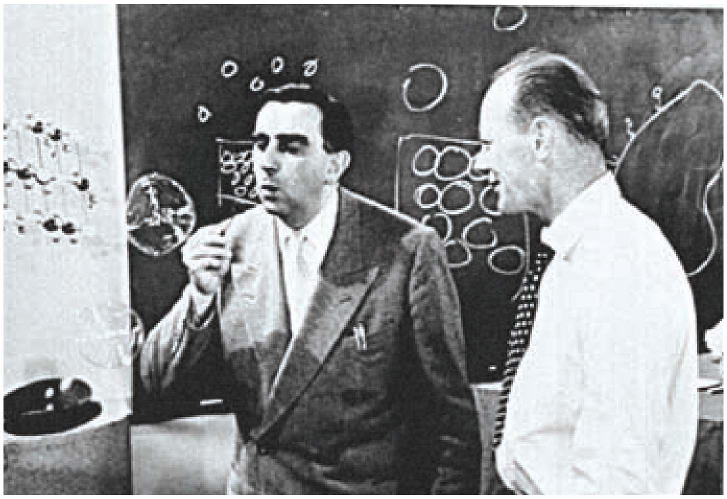
Nothing exists except atoms and empty space; everything else is opinion.

—Democritos, Greek philosopher

of Polyatomic Molecules in Degenerate Electronic States," presented the Jahn–Teller theorem. Published in the *Proceedings of the Royal Society*, this paper described how electrons force nominally symmetric molecules with more than two atoms to readjust and break the symmetry in specific ways. At the time, scientists considered this effect to be rare, but Jahn and Teller showed that it, in fact, is ubiquitous.

The Jahn–Teller theorem remains an important contribution to molecular physics research. Its significance extends through the modern physics of materials and their chemistry—from measuring spectral interactions to calculating chemical reactivity and determining molecular and condensed-matter crystal structures. For example, in 1986, the Jahn–Teller theorem was instrumental in the discovery of high-temperature superconductivity. The discoverers, Georg Bednorz and Alex Müller, chose to examine perovskites because the materials exhibited strong Jahn–Teller distortions and thus offered the promise of strong electron couplings.

Teller also explored basic atomic physics issues, most notably the two-photon decays of the metastable states of excited hydrogen and helium atoms. The resulting paper with his colleague Gregory Breit, "Metastability of Hydrogen and Helium Levels," appeared in 1940 in *Astrophysical Journal*. Their work had particular relevance to astrophysics, including cosmology, and the physics of magnetic fusion. In the corona of a star or in the early universe, when the density of atoms is low, they can exist in metastable states whose lifetimes are controlled by the two-photon rates.



Edward Teller demonstrates a physics principle in the classroom.

In 1962, Teller returned to the behavior and properties of molecules in his paper, "On the Stability of Molecules in the Thomas–Fermi Theory," which appeared in *Reviews of Modern Physics*. Written for a Festschrift, or tribute publication, to honor his friend Eugene Wigner, this concise paper addressed whether the Thomas–Fermi approximation can provide an adequate simplification to the full Schrödinger equation of quantum mechanics when applied to molecules. Teller showed that the approximation did not sufficiently capture the physics described by the more complex Schrödinger equation and thus would not predict stable, bound molecules. His result was significant in later basic analyses of the stability of matter. (See *S&TR*, April 2007, pp. 25–26.)

These discoveries, combining insights of basic atomic, molecular, and mathematical physics, continue to be important in research at Lawrence Livermore and elsewhere. From the creation of first-principles molecular dynamics simulations to the spectra of atoms and ions in gases and plasmas, Teller's legacy lives on.

—Ann Parker

Key Words: atomic physics, Edward Teller, hydrogen molecular ion, Jahn–Teller theorem, molecular physics, polymolecules, Thomas–Fermi approximation, quantum mechanics.

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